

ACS Biomaterials Science & Engineering Author Guidelines

Revised Jan 2016

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Scope & Editorial Policy

I. General Considerations

ACS Biomaterials Science & Engineering publishes work in the fields of:

1. *Modeling and informatics tools for biomaterials* – scaling methods to guide biomaterial design, predictive algorithms for structure-function, biomaterial mechanics; integrating bioinformatics with biomaterials discovery; metabolomics in the context of biomaterials.
2. *New biomaterials, bioinspired and biomimetic approaches to biomaterials* – synthesis and chemical modifications, exploiting structural hierarchy and architectural control, combinatorial strategies for biomaterials discovery, new processing modes to purify and utilize natural polymers, biophysical regulation of cell functions, controlled and bioresponsive delivery of regulatory molecules, genetic biomaterials design, synthetic biology, new composite systems.
3. *Biomaterial interfaces, biology and health* - material-biology interactions, chemical/morphological/structural communication, signaling and biological responses, health risks, toxicology, safety, calcification, corrosion and degradation of biomaterials and devices, prosthetics.
4. *Manufacturing, technology and tissues in the context of biomaterials* – regenerative medicine, tissue engineering for basic and applied studies, organ-on-a-chip, bioreactor/perfusion systems, microdevices, 3D printing, inks, BioMEMS, optics and electronics interfaces with biomaterials, systems integration

II. Types of Manuscripts

ACS Biomaterials Science & Engineering publishes four types of papers: Letters, Articles, Reviews, and Perspectives.

A. **Letters** are short articles that report results whose immediate availability to the biomaterials science and engineering community is deemed important. *Letters are restricted to 3 published pages, which is equivalent to about 2500 words or 6 double-spaced word-processed pages of text and 3-4 figures.* A brief abstract of less than 100 words should be included. Letters are intended to provide rapid communication of important results and should be written in a form that is engaging and easy to follow. The narrative should flow continuously, without separate subsections, through introductory material, followed by a sufficient outline of the experiment to allow the reader to follow what was done, results presented and described in a way that captures their essential details, and concluding remarks. Experimental details that are not essential to the understanding of the Letter, but that would be useful for those trying to reproduce the experiment, or in providing helpful additional information for experts, should be included as supporting information. Letters often will be complete publications, but follow-up publication may occasionally be justified when the research is continued and a more complete account of the work is deemed necessary. Special efforts will be made to expedite the reviewing and the publication of Letters. The time for proofreading the galley proofs is relatively short. For this reason, authors of Letters should ensure that manuscripts are in final, error-free form when submitted.

B. **Articles** should cover their subjects with thoroughness, clarity, and completeness but should be as concise as possible.

Abstracts to Articles are limited to 300 words and should summarize the significant results and conclusions. Articles are scheduled for publication in the order of acceptance within limitations of available space.

C. **Reviews** should constitute concise, yet complete, surveys of the literature written by experts for non-experts. Their purpose is to acquaint the readers of the journal with recent progress in key research areas. Reviews should be written for a more general audience of “materials scientists and engineers”, both for academic as well as industry relevance, and provide a balanced view of the topic in question. Exclusive (or near exclusive) focus on the author’s research is discouraged in Reviews. Invited and contributed Reviews will be considered for publication and will be peer-reviewed in the same manner as Letters and Articles. Authors interested in contributing a Review may submit a one-page outline for consideration. It is incumbent on authors to submit copyright permissions for material that is being reproduced from other sources.

D. **Perspectives** are generally accepted by *invitation*. Perspectives are designed to provide an enlightened appraisal of a field of research in which experts review the “state of the art” for a given topic similar to Reviews. Unlike Reviews, however, authors have editorial freedom to express their views on the strategic directions of the field of research. The Perspective series provides a forum with high visibility within the biomaterials community in industry, clinical and government research, and academia. Perspectives are peer-reviewed, contain an unreferenced abstract of 300 words or less, and include a graphical Table of Contents. Authors may choose to

divide the Perspective into sections preceded by headings. Finally, the journal recommends that authors define key words used in the Perspective and key concepts in a separate paragraph.

E. Additions and Corrections may be used to address important issues or correct errors and omissions of consequence that arise after publication of an article. They are not intended to report subsequent scientific progress or refinements, which often in part consist of reinterpreting previously published data. Additions and Corrections may be requested by the author(s) or initiated by the Editor after discussions with the corresponding author. Readers who detect errors of consequence in the work of others should contact the corresponding author of that work. All Additions and Corrections are subject to approval by the Editor, and minor corrections and additions will not be published. Additions and Corrections from authors should be submitted via the ACS Paragon Plus environment by the corresponding author for publication in the “Addition/Correction” section of the Journal. The corresponding author should obtain approval from all of the article coauthors prior to submitting an Addition and Correction, or provide evidence that such approval has been solicited. For proper formatting, see examples in a current issue of the Journal.

Addition/Corrections should consist of a submitted manuscript document file that contains the following information:

- i. The document title lines should include title, authors, affiliations and citation (including the DOI) of the original published manuscript.
- ii. The submitted addition/correction manuscript file should contain text that explains exactly what is being corrected and why. A statement should also be included indicating whether the conclusions of the work have been affected, and if so in what way.
- iii. If graphics are being corrected, the manuscript file should contain the graphics, along with captions that clearly describe the contents of the figures. The figure(s) should be labeled with numbers consistent with the figure number(s) in the original paper that is (are) being corrected.

F. Retractions. Articles may be retracted for scientific or ethical reasons. Articles that contain seriously flawed or erroneous data such that their findings and conclusions cannot be relied upon may be retracted in order to correct the scientific record. Retractions may be requested by the article author(s) or by the journal Editor(s), but are ultimately published at the discretion of the Editor. When an article is retracted, a notice of Retraction will be published containing information about the original article title, author list, and the reason for the Retraction. Retracted articles will be accompanied by the related Retraction notice and will be marked as “Retracted”. The originally published article will remain on the web except in extraordinary circumstances (e.g. where deemed legally necessary, or if the availability of the published content poses public health risks). The American Chemical Society follows guidance from the Committee on Publication Ethics (COPE) when considering retractions; for more information see: <http://publicationethics.org/>.

Preparation and Submission of Manuscripts

Web Submission

Manuscripts must be submitted via the ACS Paragon Plus Environment (<http://paragonplus.acs.org/login>). Complete instructions and an overview of the electronic

online (Web) submission process are available through the secure ACS Paragon Plus website. Authors must also submit all revisions of manuscripts via the ACS Paragon Plus Environment. The Web submission site employs state-of-the-art security mechanisms to ensure that all electronically submitted papers are secure. These same security mechanisms are also utilized throughout the peer-review process, permitting access only to editors and reviewers who are assigned to a particular paper. In order to use Web submission, authors must be able to provide electronic versions of text, graphics, and Supporting Information (if included).

The platforms and word processing packages supported by the ACS Paragon Plus Environment are listed at the *ACS Biomaterials Science & Engineering* Web edition home page via <http://pubs.acs.org/page/abseba/submission/authors.html>.

Manuscript Transfer Service

Occasionally, editors in ACS Journals feel that manuscripts are a better fit for another ACS Journal and suggest that authors consider transferring the submission. The Manuscript Transfer Service simplifies and shortens manuscript submission to another ACS journal, as all the coauthors, suggested reviewers, manuscript files, and responses to submission questions are copied to the new submission. Once authors have selected a new journal, the journal office will facilitate the transfer to that journal.

To determine if a manuscript transfer is an appropriate next step, authors are encouraged to read “[Is Manuscript Transfer Right for Me?](#)” Authors are also reminded to review [journal editorial scope statements](#) as they consider the next destination for the submission.

Requirements of the new journal may be different, so authors should also check the Author Guidelines and make any needed revisions in order to conform to those requirements. Note that transferring a manuscript is not a guarantee that the manuscript will be accepted, as the final publication decision will belong to the editor in the next journal. Please keep in mind that the reviews, reviewer identities, and decision letter will all be transferred to the new journal. For complete details, see http://pubs.acs.org/page/policy/manuscript_transfer/index.html.

ORCID

All authors are encouraged to register for an ORCID iD, a unique researcher identifier. With this standard identifier, you can create a profile of your research activities to distinguish yourself from other researchers with similar names, and make it easier for your colleagues to find your publications. Learn more at <http://www.orcid.org>.

Authors and reviewers can add their ORCID iD to, or register for an ORCID iD from, their account in ACS Paragon Plus. Submitting authors have the option to provide existing ORCID iDs for coauthors during submission, but they cannot create new ORCID iDs for coauthors.

ACS Biomaterials Science & Engineering Submission Checklist

Please check the following items before completing your submission.

Cover Letter

- A complete letter to the editor should accompany the manuscript. The required items are listed on page 5 in this document.

Title

- The title should not include words like “*Novel*”, “*New*”, or “*First*”, or numerals (Part 1, 2 etc).

Authors

- All authors and their respective current/valid email addresses should be entered into the ACS Paragon Plus Environment. Names of authors should be listed in the same sequence as they appear on the manuscript title page.
- Corresponding author is at least one senior scientist and designated with an asterisk.

Manuscript

- Manuscript [template](#) may be used, if preferred but not required. Manuscript text should appear in *one-column* format and be *double-spaced*.
- Manuscripts should be organized by sections and sub-sections. Arrange the sections as follows:
Title, Authors, Affiliations, Abstract, Keywords, Introduction, Experimental (Materials and Methods), Results, Discussion, Conclusions, Supporting information paragraph (if any), Acknowledgments (optional), References, Table of Contents graphic.

Figures and Tables

- Figures and Tables should preferably be embedded within the manuscript text, near their first mention. It is also acceptable, but not necessary, to include them at the end of the manuscript uploaded as “Graphic for manuscript” (acceptable software tif or pdf).
- Artwork should be provided at the size at which it will published in the journal, i.e., maximum 3.25 inches or 8.25 cm wide for one column.
- Each graphic should be clearly labeled and include a brief caption.
- Provide a [Table of Contents graphic](#) (TOC) at the end of the manuscript, either included in the manuscript file or uploaded separately as “Graphic for manuscript”.
- Permissions for graphics copied or adapted from previous work should be provided upon submission (uploaded as “Other files for Editor only”). In addition, correct credit lines should appear in the Figure captions.

References

- Cite references in text by unparenthesized superscript numbers. Example: ^{5-7, 9, 10}.
- The references should adhere to the format and style of *ACS Biomaterials Science & Engineering*: proper arrangement and punctuation, bold and italic font, full-page ranges.
- Include journal article titles.
- Use the CASSI abbreviations for journal titles (<http://cassi.cas.org/search.jsp>).
- Notes/comments are not accepted in the list of references.
- All author names should be included (“et al” is not accepted).
- Bibliographic information should be up to date at the time of submission.
- Provide the DOI for all journal articles, including for work published online (ASAP) but not yet in an issue.

Supporting Information, SI (if any)

- The supplementary material should be uploaded separately as “Supporting information for publication” (pdf preferred).
- A paragraph describing the SI should be included in the manuscript and placed after the Conclusions:

Supporting Information. Brief statement in nonsentence format listing the contents of the material supplied as Supporting Information.

Unpublished Work

- Upload any unpublished papers (accepted, submitted, in press, etc.) as “Supporting Information for review only”.

System Generated PDF Proof

*Last, your uploaded files (Manuscript file + Graphic(s) for manuscript) will be converted into a PDF proof. This is how the manuscript will appear when sent to reviewers. **The PDF proof must be viewed and validated before submission is completed.***

Overview

Cover Letter. A cover letter must accompany each submission. The following elements are required to be included in the letter:

- Manuscript title
- Name of the Corresponding Author
- Names(s) of all other authors
- Type of manuscript (Article, Letter, Perspective, or Review)
- A paragraph explaining the **significance** of the manuscript and why it is suitable for publication in *ACS Biomaterials Science & Engineering*
- Names and addresses of a minimum of three qualified and unbiased reviewers. A sentence listing each recommended reviewer’s expertise(s) is also required
- A statement confirming that the manuscript, or its contents in some other form, has not been published previously by any of the authors and/or is not under consideration for publication in another journal at the time of submission
- A statement confirming that *all* authors have seen and approved the submission of the manuscript
- Inform the Editor if the manuscript has previously be considered by *ACS Biomaterials Science & Engineering* or any other ACS journal
- List of graphics in need of special attention (such as permission for reproduction), if any.

Journal Publishing Agreement. A properly completed and signed Journal Publishing Agreement must be submitted for each manuscript. ACS Paragon Plus provides an electronic version of the Agreement that will be available on the **My Authoring Activity** tab of the Corresponding Author's Home page once the manuscript has been assigned to an Editor. A PDF version of the Agreement is also available, but **Authors are strongly encouraged to use the electronic Journal Publishing Agreement.** If the PDF version is used, **all pages of the signed PDF Agreement must be submitted.** If the Corresponding Author cannot or should not complete either the electronic or PDF version for any reason, another author should complete

and sign the PDF version of the form. Forms and complete instructions are available at <http://pubs.acs.org/page/copyright/journals/index.html>.

Manuscripts Submitted Elsewhere. Any closely related manuscripts that are under consideration for publication or already in press elsewhere **must** be made available for the Editor and reviewers and should be submitted as Supporting Information for Review Only.

Table of Contents Graphic. A graphic must be included with each manuscript for the Table of Contents (TOC). This graphic should capture the reader's attention and, in conjunction with the manuscript title, should give the reader a quick visual impression of the essence of the paper without providing specific results. The TOC graphic should be in the form of a structure, graph, drawing, SEM/TEM photograph, or reaction scheme. Color is acceptable and will be free of charge upon approval of the Editor. The author must submit a graphic in the actual size to be used for the TOC that will fit in an area 1.375 in. high and 3.5 in. wide (3.6 × 8.9 cm). Larger images will be reduced to fit within those dimensions. Type size of labels, formulas, or numbers within the graphic must be legible. Tables or spectra are not acceptable. Information and examples of TOC graphics can be found here:

http://pubs.acs.org/paragonplus/submission/toc_abstract_graphics_guidelines.pdf

Provide the TOC graphic upon submission of the paper as the last page of the manuscript.

Conflict of Interest Disclosure. A statement describing any financial conflicts of interest or lack thereof is published with each manuscript. During the submission process, the corresponding author must provide this statement on behalf of all authors of the manuscript. The statement should describe all potential sources of bias, including affiliations, funding sources, and financial or management relationships, that may constitute conflicts of interest (please see the [LINK: <http://pubs.acs.org/ethics>] [ACS Ethical Guidelines](#)). The statement will be published in the final article. If no conflict of interest is declared, the following statement will be published in the article: "The authors declare no competing financial interest."

Professional Ethics. In publishing only original research, ACS is committed to deterring plagiarism, including self-plagiarism. ACS Publications uses CrossCheck's iThenticate software to screen submitted manuscripts for similarity to published material. Note that your manuscript may be screened during the submission process. Further information about plagiarism can be found in Part B of the [Ethical Guidelines to Publication of Chemical Research](#).

Assistance with Improving Your Manuscript. Authors may want professional assistance with improving the English, figures or formatting in their manuscript before submission. ACS ChemWorx Authoring Services can save you time and improve the communication of research in your manuscript. You can learn more about the services offered at <http://es.acschemworx.acs.org>.

Author List. During manuscript submission, the submitting author must provide contact information (full name, email address, institutional affiliation and mailing address) for all of the co-authors. Because all of the author names are automatically imported into the electronic Journal Publishing Agreement, the names must be entered into ACS Paragon Plus in the same sequence as they appear on the first page of the manuscript. (Note that co-authors are not required to register in ACS Paragon Plus.) The author who submits the manuscript for publication accepts the responsibility of notifying all co-authors that the manuscript is being submitted. Deletion of an author after the manuscript has been submitted requires a confirming letter to the Editor-in-Chief from the author whose name is being deleted. For more information

on ethical responsibilities of authors, see the [Ethical Guidelines to Publication of Chemical Research](#).

Authors will be sent a message by e-mail acknowledging receipt of the manuscript.

Just Accepted Manuscripts

Just Accepted manuscripts are peer-reviewed, accepted manuscripts that are posted on the ACS Publications website prior to technical editing, formatting for publication, and author proofing—usually within 30 minutes to 24 hours of acceptance by the editorial office. During the manuscript submission process, Authors can choose to have their manuscript posted online as a *Just Accepted* manuscript. To ensure rapid delivery of the accepted manuscript to the Web, Authors must adhere carefully to all requirements in the journal's Author Guidelines. For further information, please refer to the *Just Accepted* FAQ, at <http://services.acs.org/pubshelp/passthru.cgi?action=kb&item=244>. Note that publishing a manuscript as *Just Accepted* is not a means by which to comply with the [NIH Public Access Mandate](#).

Preparation of Manuscripts

Authors should consult [The ACS Style Guide](#), 3rd ed. (2006, available from Oxford University Press, Order Department, 201 Evans Road, Cary, NC 27513; <http://www.oup.com/us/acs>), for format guidance.

Any author who is not fully fluent in idiomatic English is urged to obtain assistance with manuscript preparation from a fluent colleague or the ACS ChemWorx English Editing Service, as manuscripts with grammar deficiencies are sometimes handicapped during the scientific review process.

Registered trademarks should be capitalized whenever used. Trivial names for substances should not be capitalized; usually the chemical name or composition should be given in parentheses or in a footnote at the first occurrence of a trivial name.

Any unusual hazards inherent in the chemicals, equipment, or procedures used in an investigation should be clearly identified in a manuscript reporting the work.

Any animal experimentation must be approved by a local ethics committee. A statement confirming this should be included in the manuscript.

Authors are asked, if possible, to embed **graphics** in text.

Authors are encouraged, but not required, to use the online [template](#) when preparing the manuscript. If the template is not used, the text of the manuscript should be double spaced and in single-column layout.

Manuscript Organization

The manuscript document file should include the following sections and in the listed order:

Title

Titles should clearly and concisely reflect the emphasis and content of the paper. Titles are of great importance for current awareness and information retrieval and should be carefully

constructed for these purposes. Titles may not contain serial numerals (e.g. Part 1, 2, etc.) or the words “Novel”, “First” or “New”.

Authors and Affiliations

Bylines should include all those who have made substantial contributions to the work. To facilitate indexing and retrieval and for unique identification of an author, use first names, initials, and surnames (e.g., John R. Smith) or first initials, second names, and surnames (e.g., J. Robert Smith). At least one senior author must be designated with an asterisk as the author to whom correspondence should be addressed. *All authors must also be entered as co-authors in the ACS Paragon Plus Environment.*

Abstract

All manuscripts must contain an abstract, not exceeding 150 words, which should provide a succinct, informative summation of the most important results and conclusions.

Keywords

Authors are required to include four to six keywords.

Introduction

The Introduction should clearly state the aim of the work. It should provide relevant background information of research in the field. The current knowledge and the existing problem should be discussed in order to clarify the scientific interest of the submitted work. The Introduction should preferably be no longer than 2 pages.

Experimental Section

The Experimental Section should provide a clear, unambiguous description of materials, methods, and equipment in sufficient detail to permit repetition of the work elsewhere. Repetitive descriptions of a general procedure should be avoided. *Precautions for handling dangerous material or for performing hazardous procedures should be explicitly stated. In cases of animal use, approval by the local ethics committee should be stated.* Less critical experimental details should be included in the Supporting Information.

The Experimental Section should be divided into subsections (such as Materials, Methods, Results, and Discussions).

Figures, Tables, Schemes, etc., should preferably be embedded within the manuscript text, placed close to their first mention.

Conclusions

The concluding remarks must be placed under a separate Conclusions heading.

Description of the Supporting Information Material (if necessary)

If Supporting Information (SI) accompanies the submission, this section is used to describe the material. (Note, however, that the SI material should be uploaded separately.) The paragraph should be titled “Supporting Information Available” and should start with the line “The following files are available free of charge”, followed by a list of file names with brief descriptions for each.

Acknowledgments

This section may be used to acknowledge individuals, organizations, and financial support. Authors are asked to keep the acknowledgments brief.

Funding Sources.

When submitting a manuscript to the Journal via ACS Paragon Plus, the submitting author is asked to identify the funding sources for the work presented in the manuscript. Identifying funding sources is optional during submission of an original manuscript. Funding source information is required when a revised manuscript is submitted.

References

Authors should consult *The ACS Style Guide*, 3rd ed. (2006, available from Oxford University Press, Order Department, 201 Evans Road, Cary, NC 27513; <http://www.oup.com/us/acs>), for the appropriate style to use in citations of journal papers, books, and other publications.

Literature citations must be numbered in one consecutive series by order of mention in the text, with the numbers presented as unparenthesized superscripts.

Long series of references to one statement should be avoided; authors are asked to list key references only.

Footnotes or commentary notes are not accepted in the list of References.

Copies of those references that are not yet available (submitted or accepted for publication in this or other journals) must be uploaded as “Supporting information for review only”.

All references for journal articles should include the Digital Object Identifier (DOI) for convenient access, including work published online (ASAP) but not yet in an issue; see examples below (refs 1 and 3).

In literature references, journal abbreviations should be those used by Chemical Abstracts [see *Chemical Abstracts Service Source Index (CASSI) 1907–2004 Cumulative*]. The accuracy of the references is the responsibility of the authors. Because subscribers to the Web edition of the journal are now able to click on the “ChemPort” tag following each reference to retrieve the corresponding abstract at Chemical Abstracts Service, reference accuracy is critical.

Last, the following reference format must be used:

- (1) Rodell, C.B.; Kaminski, A.L.; Burdick J.A. Rational Design of Network Properties in Guest–Host Assembled and Shear-Thinning Hyaluronic Acid Hydrogels. *Biomacromolecules* **2013**, *14*, 4125–4134, DOI: 10.1021/ bm401280z.
- (2) Hoffman, A. S. In *Biomaterials Science*, 2nd ed.; Ratner, B. D., Hoffman, A. S., Schoen, F. J., Lemon, J. E., Eds.; Elsevier Academic Press: San Diego, CA, 2004; p 107.

(3) Missirlis, D.; Spatz, J.P. Combined Effects of PEG Hydrogel Elasticity and Cell-Adhesive Coating on Fibroblast Adhesion and Persistent Migration. *Biomacromolecules* **2013**, in press, DOI: 10.1021/bm4014827.

Table of Contents Graphic

The TOC graphic should be provided as the last page of the manuscript.

http://pubs.acs.org/paragonplus/submission/toc_abstract_graphics_guidelines.pdf

Guidelines for Reporting and Stewardship of NMR Data

1. NMR Text (Experimental Section):

- 1.1. The compound must be clearly identified, for example in a header at the beginning of a) the synthetic procedure or b) the summary of spectroscopic data.
- 1.2. List the nucleus being measured, any nucleus being broad-band decoupled, the solvent used (formula preferred, e.g. C₆D₆ over benzene-*d*₆), the standard used, and the field strength.
 - 1.2.1. Field strength should be noted for each spectrum, not as a comment in the general experimental section.
 - 1.2.2. The standard(s) may be specified in the general experimental section; as an example, ¹H NMR data recorded in C₆D₆ listed as “residual internal C₆D₅H (δ 7.15)”.
 - 1.2.3. Indicate solvent or peak suppression protocols used in collecting data.
- 1.3. List the probe temperature when it is accurately known; ambient probe temperature is otherwise understood.
- 1.4. Give ¹H NMR chemical shifts to two digits after the decimal point. Include the number of protons represented by the signal, peak multiplicity, and coupling constants as needed (*J* italicized, reported with up to one digit after the decimal).
 - 1.4.1. The number of bonds through which the coupling is operative, ^x*J*, may be specified by the author if known with a high degree of certainty.
 - 1.4.2. Accepted abbreviations for multiplicities and descriptors are:

s = singlet	dd = doublet of doublets
d = doublet	dt = doublet of triplets
t = triplet	td = triplet of doublets
q = quartet	br = broad signal
quint = quintet	
m = multiplet (denotes complex pattern)	

- 1.5. Chemical shifts should be listed consistently in a single article, starting either from downfield to upfield or vice-versa. Please consult the Author Guidelines for preferred formatting for each journal.
- 1.6. Assign peak identities under the following circumstances:
 - 1.6.1. Non-decoupled or equivalent spectra have been collected (^{13}C , ^{31}P , etc).
 - 1.6.1. 2-D experiments have been performed.
 - 1.6.2. Unambiguous assignment is possible without additional experiments, such as in the case of an organometallic metal-hydride ^1H signal, PF_6 vs. MPPh_3 ^{31}P signal, etc.
- 1.7. Give ^{13}C chemical shifts to one digit after the decimal point, unless an additional digit will help distinguish overlapping peaks.
 - 1.7.1. Include peak multiplicities for ^1H -coupled ^{13}C NMR spectra, or for signals in ^1H -decoupled spectra that are coupled to other magnetically active nuclei.
 - 1.7.2. A ^{13}C NMR signal will be considered a singlet if the multiplicity is not assigned.
 - 1.7.3. Only rarely is a true multiplet observed in a $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum. However, a certain region may contain a group of unresolved peaks or signals.
- 1.8. Mention of unobserved resonances is encouraged.

Example 1 (no 2-D data collected):

($\eta^5\text{-C}_5\text{Me}_5\text{Co}$) $_2$ - μ -(η^4 : η^4 - C_9H_{10}) (**1**): ^1H NMR (C_6D_6 , 400 MHz): δ -0.53 (s, 1H), 0.72 (d, 1H, J = 4.0 Hz), 0.98 (s, 1H), 1.58 (s, 15H), 1.62 (s, 3H), 1.73 (s, 15H), 1.95 (d, 1H, J = 4.0 Hz), 5.62 (t, 1H, J = 4.0 Hz), 6.00 (t, 1H, J = 4.0 Hz). $^{13}\text{C}\{^1\text{H}\}$ NMR (C_6D_6 , 400 MHz): δ 10.2, 10.6, 17.4, 38.3, 51.5, 54.2, 60.6, 80.8, 81.0, 88.0, 88.7.

Example 2 (2-D data collected):

Silvestrol (**2**): ^1H NMR (CDCl_3 with 0.05% v/v TMS, 400 MHz): δ_{H} 7.10 (2H, d, J = 8.9 Hz, H2' and H6'), 7.03-7.07 (3H, m, H3'', H4'' and H5''), 6.83-6.85 (2H, m, H2'' and H6''), 6.66 (2H, d, J = 8.9 Hz, H3' and H5'), 6.42 (1H, d, J = 1.8 Hz, H5), 6.26 (1H, d, J = 1.7 Hz, H7), 5.18 (1H, s, H1'''), 5.01 (1H, d, J = 6.6 Hz, H1), 4.52 (1H, s, H2'''), 4.27 (1H, d, J = 14.2 Hz, H3), 4.15 (1H, br d, J = 11.2 Hz, H4'''), 4.05 (1H, t, J = 11.2 Hz, H3b'''), 3.88 (1H, J = 14.3, 6.8 Hz, H2), 3.86 (3H, s, OCH_3 8), 3.69 (3H, s, OCH_3 4'), 3.64 (3H, s, COOCH_3 2), 3.49 (3H, br s, H5''' and H6'''), 3.43-3.47 (1H, overlapped, H3a'''), 3.45 (3H, s, OCH_3 2'''). ^{13}C NMR (CDCl_3 , 125 MHz): δ_{C} 170.6 (s, COCH_3 2), 160.6 (s, C4a), 160.0 (s, C6), 158.8 (s, C4'), 157.1 (s, C8), 136.7 (s, C1''), 129.0 (d, C2' and C6'), 127.8 (d, C2'', C3'', C5'' and C6''), 126.6 (d, C4''), 126.3 (s, C1'), 112.7 (d, C3' and C5'), 109.6 (s, C8a), 101.9 (s, C3a), 95.2 (d, C2'''), 94.0 (d, C1'''), 93.9 (d, C7), 93.4 (s, C8b), 92.9 (d, C5), 79.7 (d, C1), 70.7 (d, C5'''), 68.3 (d, C4'''), 63.3 (t, C6'''), 59.0 (t, C3'''), 55.9 (q, OCH_3 8), 55.1 (q, OCH_3 4'), 55.0 (d, C3; q, OCH_3 2'''), 52.1 (q, COCH_3 2), 50.3 (d, C2).

Note

Broad peaks between δ_{H} 1.5 to 3.0 ppm and at δ_{H} 3.79 ppm correspond to the protons of the OH groups on C-1, C-8, C-5''' and C-6''', which disappeared after D_2O exchange.

Example 3:

(*E,E*)-3,7,11-Trimethyl-2,6,10-dodecatrien-1-yl diphosphate (Farnesyl diphosphate, FPP, **3**): ^1H NMR (D_2O , 300 MHz): δ 1.61 (s, 6H), 1.68 (s, 3H), 1.72 (s, 3H), 2.17-1.99 (m, 8H), 4.45 (d of d, 2H, $J_{\text{H,H}}$ = 6 Hz, $J_{\text{P,H}}$ = 6 Hz), 5.23-5.15 (m, 2H), 5.46 (t, 1H, J = 6 Hz). ^{13}C NMR (D_2O , 75

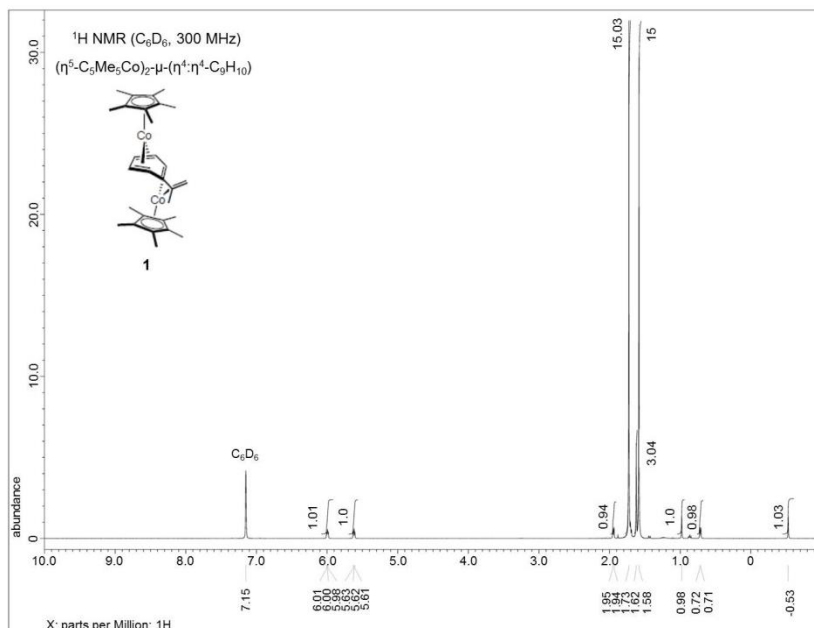
MHz): δ 16.3, 16.6, 17.9, 25.9, 27.0, 27.2, 40.1, 40.2, 63.2, 120.5, 124.8, 125.1, 131.6, 135.9, 142.8. ^{31}P NMR (D_2O , 121.5 MHz): δ -6.56 (d, 1P, $J_{\text{P,P}} = 21.9$ Hz), -9.89 (d, 1P, $J_{\text{P,P}} = 21.9$ Hz).

2. NMR Spectra (Supporting Information):

Submission of spectra (.doc, .docx, .txt, .pdf, .tif) is strongly recommended for all new and/or key compounds. When submitting spectra, please consider the following guidelines:

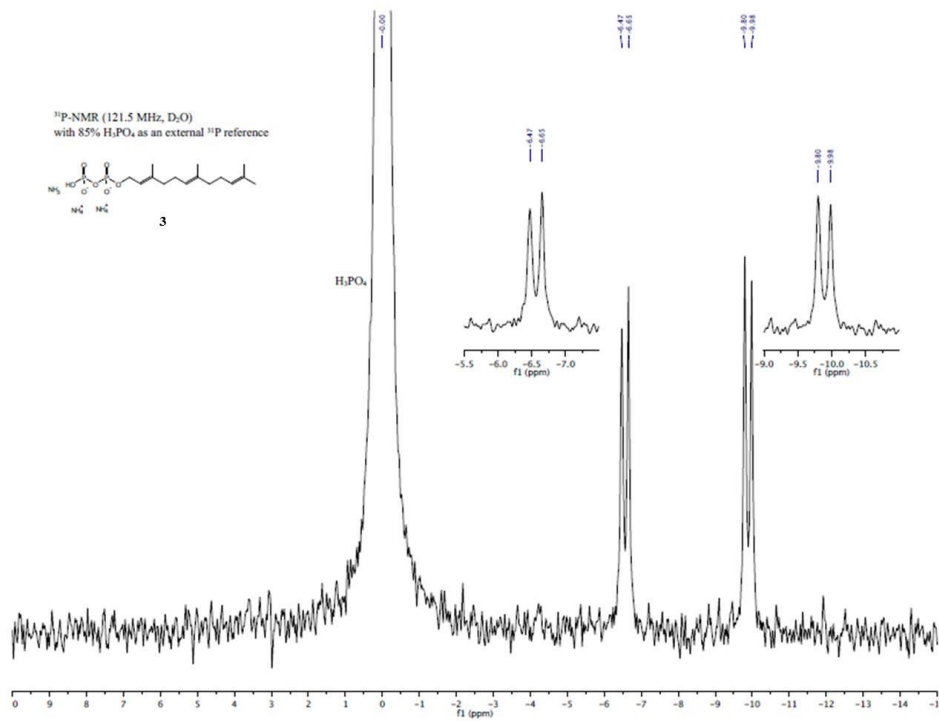
- 2.1. A caption should be included on the spectrum, noting the nucleus being measured, the solvent (formula preferred, e.g. C_6D_6 over benzene- d_6) and the field strength.
- 2.2. A representation of the compound should be included on the spectrum – please use ChemDraw or a related program. The compound identifier used in the manuscript should be included.
- 2.3. The largest peak in the ^1H NMR spectrum should normally arise from the compound, not the solvent.
- 2.4. All peaks in the ^1H NMR spectrum should be integrated. Chemical shift values should be included.
- 2.5. The solvent peak should be clearly labeled on the spectrum.
- 2.6. All peaks should be visible on the spectrum. Insets are encouraged to show expanded regions. At minimum, the spectral window should be -1 ppm to 9 ppm for ^1H NMR and -10 ppm to 180 ppm for ^{13}C NMR.
- 2.7. Font should be clear and large enough to read (minimum of 10 point). Horizontal orientation is preferred for spectra.

Example 1:



Example 2:





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General Considerations. Remove all color from graphics, except for those graphics that you would like to have considered for publication in color (see Color section below for details).

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The quality of the illustrations in your paper depends on the quality of the artwork originals you provided. Figures cannot be modified or enhanced by the journal production staff. **Artwork should be provided at the size at which it will be published in the journal.** To ensure good quality production in the journal, a copy of each graphic should be printed (at the desired size in the final published version) from a high-quality laser printer (600 dpi or higher) to verify that all parts of the artwork are clear and legible. Any changes to the artwork (including size changes) must be made in the drawing program that was used to create the artwork, and the revised artwork reimported into the manuscript.

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	single (preferred)	double
width		
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maximum	8.25 cm (3.25 in.)	17.78 cm (7 in.)
maximum depth	24 cm (9.5 in.)	24 cm (9.5 in.)

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bond spacing	18% of width
fixed length	14.4 pt (0.508 cm, 0.2 in.)
bold width	2.0 pt (0.071 cm, 0.0278 in.)
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margin width	1.6 pt (0.056 cm, 0.0222 in.)
hash spacing	2.5 pt (0.088 cm, 0.0347 in.)

(2) As text settings select:

font	Arial/Helvetica
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(3) Under the preferences choose:

units	points
tolerances	5 pixels

(4) Under page setup choose:

Paper	US Letter
Scale	100%

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(6) Embolden compound numbers, but not atom labels or captions.

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- Use Helvetica or Arial type for lettering.
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